The Fermi-Pasta-Ulam paradox, Anderson Localization problem and the the generalized diffusion approach

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Abstract

The goal of this paper is two-fold. First, based on the interpretation of a quantum tight-binding model in terms of a classical Hamiltonian map, we consider the Anderson localization (AL) problem as the Fermi-Pasta-Ulam (FPU) effect in a modified dynamical system containing both stable and unstable (inverted) modes. Delocalized states in the AL are analogous to the stable quasi-periodic motion in FPU; whereas localized states are analogous to thermalization, respectively. The second aim is to use the classical Hamilton map for a simplified derivation of *exact* equations for the localization operator $H(z)$. The letter was presented earlier [J.Phys.: Condens. Matter **14** (2002) 13777] treating the AL as a generalized diffusion in a dynamical system. We demonstrate that counter-intuitive results of our studies of the AL are similar to the FPU counter-intuitivity.

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I. INTRODUCTION

Half a century ago two celebrated papers were published temporally close to each other which gave birth to two fundamental directions of theoretical physics. In 1955 the *Fermi-Pasta-Ulam* (hereafter, FPU) *paradox* was formulated [1, 2] which suggested the nonequipartition of energy among normal modes of an anharmonic atomic chain. This phenomenon is closely connected with the problems of ergocidity, integrability, chaos and stability of motion [2, 3]. A few years later, in 1958, *Anderson* [4] suggested the possibility of electron localization (AL) in a random system, provided that the disorder is sufficiently large. This idea is one of the foundations for the understanding the electronic properties of disordered systems [5]. From a more general point of view, this idea implies the absence of wave diffusion in a random medium as a universal feature of stochastic processes. Unlike the AL problem, where the stochasticity was explicitly introduced into consideration through random potentials, the FPU considers the stochasticity as a non-trivial effect in the dynamics of nonlinear systems, since a strong chaos behaviour can be observed even in a system with several degrees of freedom.

Despite the fact that the FPU paradox can be reformulated analogously to the AL problem in terms of waves (ineraction of normal modes which are characterized by their wave number k), their conceptual similarity has not been noticed so far. In fact, *localization*, even when mentioned in the FPU literature, is not associated with disorder; usually this means that the energy initially placed in a low-frequency normal mode k_0 of the linear problem stay almost completely locked within a few modes neighboring the k_0 mode. The localization in k-space of normal modes [6] or analogous energy localization in the FPU chain [7] are typically considered here. Sometimes the AL and FPU are mentioned together, but as *independent* and even competing processes. In particular, energy transport in binary isotropically disorded nonlinear FPU chains was considered [8] with the competition between localization (a *disorder* effect) and mode transitions (a *nonlinearity* effect). Notice also that the close connection between the nonlinear dynamics and the AL was established for nonlinear systems with a much smaller number of freedom degrees than in the FPU problem. Thus, it was shown that the quantum kicked rotor model [9, 10] can be mapped onto the AL model. On the other hand, the quantum kicked rotor serves as the starting point of the systematic analysis of the quantum dynamics of classically chaotic dynamical

systems.

Our purpose is to establish a *close connection* between the two fundamental problems. That is, the AL is nothing else but the FPU effect in a modified dynamical system with interacting normal modes. Besides, the delocalized states in the AL problem are analogous to the stable quasi-periodic motion (recurrence in the FPU problem) and, respectively, the localized states are similar to the *thermalization* (motion instability) in the FPU. Our FPU modification includes: (i) non-trivial change of the mode ensemble. In the FPU without interactions all normal modes are stable. In contrast, in the AL both stable and unstable (*inverted*) modes also exist. (ii) a modified mode interaction: the stochasticity in the AL is introduced directly, through random forces *linear* in coordinates and rather indirectly, through nonlinear terms in the dynamical equations.

A critical comparison of the AL problem and the FPU paradox is the more useful since the former turned out to be also a paradox. Indeed, in recent years, the conflicting situation was established here: (a) experimental results contradict the generally-accepted theory [5, 11], whereas (b) the analytical theory contradicts numerical simulations [12, 13]. Despite such a clear conflict, the results of our *exact* analytical theory [14, 15, 16] are considered as highly unexpected in the Anderson community [17, 18, 19, 20] since they contradict the generally-accepted results of the scaling theory [21] and numerical modeling [12]. In particular, doubts are expressed about our conclusion on the existence of the metal-insulator transition in the two dimensional (2D) disordered system of noninteracting electrons (which does not contradict real experimental data [5, 11]) and that the Anderson transition is of the first-order (localized and conducting state co-exist). The latter statement is a clear example of a counter-intuitive prediction. Appearance of highly unexpected results is typical for such counter-intuitive (paradox) problems such as the AL and FPU.

In this paper, we employ the main results of our analytical method [14, 15, 16] and treat the AL as generalized diffusion in a dynamical system. The random forces impose random walk amplitudes (the dynamics is bounded in the phase space for unperturbed system) which can lead to the diffusion divergence. The diffusion problem with random forces linear in the coordinates can be exactly solved. Moreover, the diffusion concept permits to connect the AL and FPU problems. As is well-known [10], the equations for nonlinear dynamical systems can under certain conditions describe pseudo-random walks which leads to the diffusion behaviour and diffusion increase in mean energy (i.e. divergence).

We shall employ also the interpretation of the Schrödinger equation (quantum tight-binding model) in terms of the classical Hamiltonian map [22, 23, 24]. As a result, the problem can be reformulated in terms of interacting mode dynamics which opens the opportunity for the detailed comparison of AL with FPU. It should be stressed that ideas [22, 23, 24] allow to simplify considerably the mathematical formalism used earlier [14, 15, 16]. This is important in the light of the recent criticism [17, 19] that the *engineering language* (signal theory) of the mentioned formalism (input and output signals, filter function, etc.) is new for the AL community. In this paper we suggest a compact derivation of the main feature of the disordered system - the localization operator $H(z)$ [16].

The structure of the paper is as follows. In Section II A we explain how the one-dimensional tight-binding model with diagonal disorder can be presented in terms of the classical two-dimensional Hamiltonian map for normal or inverted oscillators. In Section II B we present the equations for arbitrary dimensions. We show that delocalized states, in general, correspond to the statistically bound trajectories, whereas localized states to unbound trajectories, respectively. The trajectory type depends on the excited mode (normal or inverted). We show in Section II C that statistically unbound trajectories can be treated in terms of a *generalized diffusion*, with exactly predicable properties. As a result, we arrive in Section II D at the definition of the localization operator $H(z)$. In Section III a possible comparison of the AL and FPU problems is discussed. It is shown that the AL treatment in terms of the classical Hamiltonian map results in a paradox demonstrating the counter-intuitive nature of this problem. The results [14, 15, 16] are compared with those for the FPU and their detailed similarities are analyzed.

II. ANDERSON LOCALIZATION AND CLASSICAL HAMILTONIAN MAP

A. Cauchy problem and classical Hamiltonian map for the one-dimensional case

As is well known, in order to determine the Lyapunov exponent γ (which is the inverse of the localization length, $\xi = 1/\gamma$) and the phase diagram (the areas of the localized and delocalized states), the Cauchy problem with fixed initial conditions has to be solved [12, 14, 19, 25]. For illustration, the 1D Schrödinger equation

$$\psi_{n+1} + \psi_{n-1} = E\psi_n - \varepsilon_n\psi_n \tag{1}$$

with random potentials ε_n can be presented as a recursive relation

$$\psi_{n+1} = E\psi_n - \psi_{n-1} - \varepsilon_n\psi_n. \tag{2}$$

The treatment of one of the spatial coordinates as a temporal variable (discrete time n) is a standard approach in chaos theory [26] which opens the way to the dynamical interpretation. Taking into account the so-called *causality principle* [14, 16], the latter equation permits an exact stochastic analysis. Indeed, it is easy to see that in the Cauchy problem (with fixed initial conditions for ψ_1 and ψ_0), eq.(2), ψ_2 is a function of ε_1, ψ_3 is a function of ε_2,ε_1, etc (a *causality*). That is both amplitudes ψ_n and ψ_{n-1} on the rhs of eq.(2) are statistically independent of ε_n and can be averaged separately (causality principle):

$$\langle\psi_{n+1}\rangle = (E - \langle\varepsilon_n\rangle)\langle\psi_n\rangle - \langle\psi_{n-1}\rangle, \tag{3}$$

$$\begin{aligned}\langle\psi_{n+1}^2\rangle = (E^2 - 2E\langle\varepsilon_n\rangle + \langle\varepsilon_n^2\rangle)\langle\psi_n^2\rangle - \\ -2(E - \langle\varepsilon_n\rangle)\langle\psi_n\psi_{n-1}\rangle + \langle\psi_{n-1}^2\rangle.\end{aligned} \tag{4}$$

The causality principle can be used only (a) for the recursive relation for the Cauchy problem and (b) when on-site potentials are independently distributed ($\langle\varepsilon_n\varepsilon_{n'}\rangle = \sigma^2\delta_{n,n'}$) but not for the Dirichlet problem, correlated potentials, etc.

To study the origin of localized/delocalized states, we use a simple approach [22, 23, 24] based on the interpretation of a quantum tight-binding model, eq.(2), with diagonal disorder in terms of the classical two-dimensional Hamiltonian map. The difference equation (2) is reduced to a discrete transform with a simple physical interpretation. Let us write the second-order equation as a set of two first-order equations. Assume $q_n = \psi_n$ and $p_n = \psi_{n+1} - \psi_n$ for $E \geq 0$; whereas $q_n = -\psi_n$ and $p_n = -(\psi_{n+1} - \psi_n)$ as $E < 0$. The obtained equation set reads

$$p_{n+1} = p_n - \omega^2 q_n - \varepsilon_n q_n, \tag{5}$$

$$q_{n+1} = q_n + p_{n+1}, \tag{6}$$

where $\omega^2 = 2 - |E|$.

As is shown [26], the discrete transform (5), (6) can be connected with the equivalent differential equation of the Hamilton dynamics with the Hamiltonian (kicked oscillator)

$$\mathcal{H} = \frac{p^2}{2} + \frac{\omega^2 q^2}{2} + \frac{\varepsilon(t)q^2}{2}\sum_n \delta(t - n\Delta t). \tag{7}$$

It defines the system with the unperturbed Hamiltonian for an oscillator affected by a periodic sequence of a kicks (δ-pulses) with the period Δt. Discrete transform arises when magnitudes of coordinate and impulse are considered with a discrete time increment Δt and correspondingly with a discrete time index n (discrete time).

Dependent on the ω^2 sign, there exist two cases. For $|E| < 2$, corresponding to the solutions inside the band in the unperturbed system, we obtain a normal (stable) oscillator with $\omega^2 > 0$. On the contrary, the energies outside the band, $|E| \geq 2$, are associated with inverted (unstable) oscillators with $\omega^2 \leq 0$. Without disorder $\varepsilon_n \equiv 0$ and delocalized quantum states correspond to a normal oscillator and trajectories bound in the classical (p, q) space as $n \to \infty$ [23]. Simple characteristics of the dynamical system q_n^2 or p_n^2 are bound, respectively. Contrary, an inverted oscillator describes non-physical solutions outside the band which are now unbound in the classical phase space; the q_n^2 magnitude is divergent as $n \to \infty$.

When disorder is introduced, the situation changes qualitatively. Random kicks for a normal oscillator lead to the random amplitude walks. The oscillatory motion remains since the average $\langle q_n \rangle$ remains bound as $n \to \infty$. For a random amplitude walk long trajectories in the classical phase space (p, q) are possible which can be treated as diffusion [16]. This is characterized by a typical parameter divergence: $\langle q_n^2 \rangle \to \infty$ as $n \to \infty$. Since these trajectories correspond in 1D to the localized states, these can be considered as statistically unbound. In the case of the inverted oscillator the amplitude increases exponentially (in the model with Hamiltonian eq.(7)) between successive kicks, but the force linear in coordinates is able to change a coordinate sign.

Use of the diffusion terminology is quite justified here. Indeed, to detect the diffusion, it is sufficient to demonstrate the divergence of the second moment of the amplitude q_n and to establish its time-dependence, the function $f(n)$ in $\langle q_n^2 \rangle = f(n)$. The divergence of the second moment defines the conditions of the diffusion appearance. For a *normal diffusion* the mean square displacement is linear in time, $\langle q_n^2 \rangle \propto n$. The notion of an *anomalous diffusion* [27, 28] derives from the fact that the mean square displacement may be anomalously diffusive, $\langle q_n^2 \rangle \propto n^\alpha$ ($\alpha \neq 1$), i.e. nonlinear in time (power-law divergence). The quantity $\langle q_n^2 \rangle = \langle \psi_n^2 \rangle$ in eq.(2) was calculated analytically [14, 25]: $\langle q_n^2 \rangle \propto \exp(2\gamma n)$ with $\gamma \geq 0$ for an arbitrary E value, provided $\sigma > 0$. In this case the *generalized diffusion* (exponential divergence) takes place. The appearance of the localization in the approach

based on eq. (2) is equivalent to the appearance of diffusion. Respectively, the well-known statement that in one dimension all states are localized at any level of disorder, is equivalent to the statement on the diffusion character of all solutions of eq.(2) in 1D for $\sigma > 0$.

B. Classical Hamiltonian map for D-dimensional case

The above-discussed statement of the problem can be naturally generalized for an arbitrary dimension D; this idea was mentioned but not realized in Ref. [24]. The phase diagram of the system with metal-insulator transition should be obtained in the thermodynamical limit (the infinite system). Let us consider the semi-infinite system, or an infinite system with a boundary, where the index $n \equiv m_D \geq 0$, but all $m_j \in (-\infty, \infty)$, $j = 1, 2, \ldots, p$, with $p = D - 1$. We combine indices in the form of a vector $\mathbf{m} = \{m_1, m_2, \ldots, m_p\}$. The boundary which is the layer $n = 0$ defines the preferential direction (the axis n).

The Schrödinger equation can be rewritten as a recursion equation (in terms of the discrete-time n)

$$\psi_{n+1,\mathbf{m}} = (E - \varepsilon_{n,\mathbf{m}})\psi_{n,\mathbf{m}} - \psi_{n-1,\mathbf{m}} - \sum_{\mathbf{m}'} \psi_{n,\mathbf{m}'}. \tag{8}$$

Summation over $\mathbf{m}'$ runs over the nearest neighbours of the site $\mathbf{m}$. The on-site potentials $\varepsilon_{n,m}$ are independently and identically distributed. We assume hereafter existence of the two first moments, $\langle \varepsilon_{n,\mathbf{m}} \rangle = 0$ and $\left\langle \varepsilon^2_{n,\mathbf{m}} \right\rangle = \sigma^2$, where the parameter σ characterizes the disorder level.

Let us perform the Fourier transform:

$$\varepsilon_n(\mathbf{k}) = \sum_{\mathbf{m}} \varepsilon_{n,\mathbf{m}} e^{i\mathbf{km}}, \tag{9}$$

$$\psi_n(\mathbf{k}) = \sum_{\mathbf{m}} \psi_{n,\mathbf{m}} e^{i\mathbf{km}}. \tag{10}$$

The relation for similar random quantities, , $\langle \varepsilon_{n,\mathbf{m}} \rangle = 0$, $\langle \varepsilon_{n,\mathbf{m}} \varepsilon_{n',\mathbf{m}'} \rangle = \sigma^2 \delta_{n,n'} \delta_{\mathbf{m},\mathbf{m}'}$, leads to

$$\langle \varepsilon_n(\mathbf{k}) \rangle = 0, \tag{11}$$

$$\langle \varepsilon_n(\mathbf{k}) \varepsilon^*_{n'}(\mathbf{k}') \rangle = (2\pi)^p \sigma^2 \delta_{n,n'} \delta(\mathbf{k} - \mathbf{k}'). \tag{12}$$

As a result of the Fourier transform, the Schrödinger equation (8) transforms into the equation set for the mode dynamics, enumerated by the index $\mathbf{k}$,

$$\psi_{n+1}(\mathbf{k}) = \mathcal{L}(\mathbf{k})\psi_n(\mathbf{k}) - \psi_{n-1}(\mathbf{k}) - \int \frac{d^p\mathbf{k}_1}{(2\pi)^p} \varepsilon_n(\mathbf{k} - \mathbf{k}_1)\psi_n(\mathbf{k}_1). \tag{13}$$

Here

$$\mathcal{L}(\mathbf{k}) = E - 2\sum_{j=1}^{p=D-1}\cos(k_j), \tag{14}$$

with fixed initial conditions $\psi_0(\mathbf{k})$ and $\psi_1(\mathbf{k})$.

A comparison of eq.(13) with its 1D analog, eq.(2), demonstrates that the dynamics of the multi-dimensional system can be reduced to the dynamics of the multi-oscillatory system. The frequencies of these oscillators are defined by the relation $\omega(\mathbf{k})^2 = 2 - |\mathcal{L}(\mathbf{k})|$. That is, one can distinguish, as before, normal oscillators with $|\mathcal{L}(\mathbf{k})| < 2$ and inverted oscillators with $|\mathcal{L}(\mathbf{k})| \geq 2$. As we have shown [16], the condition $|\mathcal{L}(\mathbf{k})| < 2$ without perturbation corresponds to delocalized states inside the band; and contrary, $|\mathcal{L}(\mathbf{k})| \geq 2$ corresponds to the solution outside the band. In other words, the connection between the classical oscillator type (normal or inverted) and the quantum-mechanical solution remains also for arbitrary dimensions. However, there is also an important difference between the 1D and ND systems: in the former case the energy magnitude determines uniquely the oscillator type. The terms with a random force describe only the oscillator's stochastic self-interaction, due to its linear dependence, $-\varepsilon_n q_n$ in eq.(5), the oscillator cannot be stopped, $q = p = 0$.

In contrast, in the multi-dimensional case the energy E no longer determines uniquely the system's state, the fixed initial conditions $\psi_0(\mathbf{k})$ and $\psi_1(\mathbf{k})$ define simultaneously the type and number of initially excited oscillators, among which can be found both normal and inverted oscillators. The integral in eq.(13) corresponding to a random force, describes now the stochastic interaction between oscillators. That is, knowledge of the 1D system is *not* sufficient for the description of multi-dimensional systems; as we demonstrate below, fundamentally new effects arise here.

Using the *causality principle* [14, 16], the equation for the first momentum of a random amplitude $\langle\psi_n(\mathbf{k})\rangle$ is quite trivial:

$$\langle\psi_{n+1}(\mathbf{k})\rangle = \mathcal{L}(\mathbf{k})\langle\psi_n(\mathbf{k})\rangle - \langle\psi_{n-1}(\mathbf{k})\rangle. \tag{15}$$

It is easy to see that for unstable modes, $|\mathcal{L}(\mathbf{k})| \geq 2$, even the first moments are divergent, $|\langle\psi_n(\mathbf{k})\rangle| \to \infty$, as $n \to \infty$. Its analog in the classical phase space (p, q) corresponds to unbound trajectories.

Since we associate the appearance of localized states with unbound trajectories for classical oscillators, it is easy to formulate the necessary (but not sufficient) condition for the

appearance with disorder of the delocalized states: the initial conditions should correspond to excitation of normal oscillators only, i.e. the amplitudes $\psi_0(\mathbf{k})$ and $\psi_1(\mathbf{k})$ are nonzero only for modes with $|\mathcal{L}(\mathbf{k})| < 2$. This coincides with the statement [16] based on different ideas. Under this condition the dynamics of the first moments is bound for all modes, $|\langle\psi_n(\mathbf{k})\rangle| < \infty$ as $n \to \infty$. However, this condition is not sufficient, since the localized states as it was illustrated for the 1D case, correspond in general to *statistically unbound trajectories*, $\langle|\psi_n(\mathbf{k})|^2\rangle \to \infty$ as $n \to \infty$. That is, the search for the sufficient condition for the excistence of the delocalized states is reduced to the solution of equations for the *second moments* of the random amplitudes [14, 16].

C. Equations for second moments

Divergence of the second moments is a typical diffusion behaviour; an observation of such a diffusion dynamics indicates directly the presence of the localized states, and vice versa. An easy criterium of a diffusion is the behaviour of the squared coordinate for all oscillators

$$U_n = \int \frac{d^p\mathbf{k}}{(2\pi)^p}\langle|\psi_n(\mathbf{k})|^2\rangle. \tag{16}$$

To detect the diffusion, it is sufficient to demonstrate divergence of the function U_n as $n \to \infty$.

Let us define the second moments by the relations:

$$x_n(\mathbf{k}) = \langle|\psi_n(\mathbf{k})|^2\rangle = \langle\psi_n(\mathbf{k})\psi_n^*(\mathbf{k})\rangle, \tag{17}$$

$$y_n(\mathbf{k}) = \frac{1}{2}[\langle\psi_n(\mathbf{k})\psi_{n-1}^*(\mathbf{k}) + \psi_n^*(\mathbf{k})\psi_{n-1}(\mathbf{k})\rangle]. \tag{18}$$

One gets

$$U_n = \int \frac{d^p\mathbf{k}}{(2\pi)^p}x_n(\mathbf{k}). \tag{19}$$

Using the causality principle (see details in Ref.[14, 16])) for eq.(13), one gets immediately for the non-zero average quantities:

$$\begin{aligned}\langle|\psi_{n+1}(\mathbf{k})|^2\rangle = \mathcal{L}^2(\mathbf{k})\langle|\psi_n(\mathbf{k})|^2\rangle + \langle|\psi_{n-1}(\mathbf{k})|^2\rangle \\ -\mathcal{L}(\mathbf{k})\langle[\psi_n(\mathbf{k})\psi_{n-1}^*(\mathbf{k}) + \psi_n^*(\mathbf{k})\psi_{n-1}(\mathbf{k})\rangle \\ + \int\int \frac{d^p\mathbf{k}_1}{(2\pi)^p}\frac{d^p\mathbf{k}_2}{(2\pi)^p}\langle\varepsilon_n(\mathbf{k}-\mathbf{k}_1)\varepsilon_n^*(\mathbf{k}-\mathbf{k}_2)\rangle\langle\psi_n(\mathbf{k}_1)\psi_n^*(\mathbf{k}_2)\rangle.\end{aligned} \tag{20}$$

Taking into account properties of random potentials, eq.(12), one gets for $n \geq 1$:

$$x_{n+1}(\mathbf{k}) = \mathcal{L}^2(\mathbf{k})x_n(\mathbf{k}) + x_{n-1}(\mathbf{k}) - 2\mathcal{L}(\mathbf{k})y_n(\mathbf{k}) + \sigma^2 U_n. \tag{21}$$

Notice that the last term in eq.(21) does not depend on $\mathbf{k}$, i.e. the noise equally affects *all* modes. The noise intensity is described by $\sigma^2 U_n$, where U_n was defined in eq.(19). Analogously, the complementary equation is derived

$$y_{n+1}(\mathbf{k}) + y_n(\mathbf{k}) = \mathcal{L}(\mathbf{k})x_n(\mathbf{k}). \tag{22}$$

Let us perform now the Z-transform:

$$X(z,\mathbf{k}) = \sum_{n=1}^{\infty} \frac{x_n(\mathbf{k})}{z^n}, \tag{23}$$

$$Y(z,\mathbf{k}) = \sum_{n=1}^{\infty} \frac{y_n(\mathbf{k})}{z^n}, \tag{24}$$

$$U(z) = \sum_{n=1}^{\infty} \frac{U_n}{z^n}. \tag{25}$$

Takin into account eq.(19), one gets easily

$$U(z) = \int \frac{d^p\mathbf{k}}{(2\pi)^p} X(z,\mathbf{k}). \tag{26}$$

The Z-transform of eqs.(21), (22) leads to the relations containing the initial conditions

$$[z - z^{-1} - \mathcal{L}^2(\mathbf{k})]X(z,\mathbf{k}) + 2\mathcal{L}(\mathbf{k})Y(z,\mathbf{k}) = \tag{27}$$
$$x_1(\mathbf{k}) + z^{-1}x_0(\mathbf{k}) + \sigma^2 U(z),$$

$$(z+1)Y(z,\mathbf{k}) - \mathcal{L}(\mathbf{k})X(z,\mathbf{k}) = y_1(\mathbf{k}). \tag{28}$$

It is easy to find that

$$\frac{(z-1)}{(z+1)}[(z+1)^2/z - \mathcal{L}^2(\mathbf{k})]X(z,\mathbf{k}) = \lambda(z,\mathbf{k}) + \sigma^2 U(z), \tag{29}$$

where $\lambda(z,\mathbf{k}) = 2\mathcal{L}(\mathbf{k})y_1(\mathbf{k})/(z+1) + x_0(\mathbf{k}) + x_1(\mathbf{k})/z$. Taking into account the definition (26), eq.(29) is the integral equation, but with a simple structure.

The initial conditions for moments are easily expressed through $\psi_0(\mathbf{k})$, $\psi_1(\mathbf{k})$. The trivial result is that if any mode with the wave vector $\mathbf{k}_0$ enters the initial conditions (i.e. at least one of the two quantities $\psi_0(\mathbf{k})$, $\psi_1(\mathbf{k})$ is non-zero), the quantity $\lambda(z,\mathbf{k}_0)$ is also non-zero for this mode. This will be used in the further analysis.

D. Localization operator

Let us assume for the beginning that $\sigma = 0$, i.e. there is no disorder in eq.(29), and use the relevant solution $X^{(0)}(z, \mathbf{k})$ for the calculation of the squared coordinate, eq.(26). Thus, one gets

$$U^{(0)}(z) = \frac{(z+1)}{(z-1)} \int \frac{d^p\mathbf{k}}{(2\pi)^p} \frac{\lambda(z, \mathbf{k})}{[(z+1)^2/z - \mathcal{L}^2(\mathbf{k})]}. \tag{30}$$

For $\sigma \neq 0$ the solution reads

$$U(z) = H(z)U^{(0)}(z). \tag{31}$$

Here $H(z)$ is the localization operator

$$\frac{1}{H(z)} = 1 - \sigma^2 \frac{(z+1)}{(z-1)} \int \frac{d^p\mathbf{k}}{(2\pi)^p} \frac{1}{[(z+1)^2/z - \mathcal{L}^2(\mathbf{k})]}. \tag{32}$$

Using the convolution property for the Z-transform [14, 16], one gets

$$U_n = \sum_{l=1}^{n} U_l^{(0)} h_{n-l}, \tag{33}$$

where h_n is the result of the inverse Z-transform of the localization operator $H(z)$.

As was mentioned, the necessary condition for the existence in the presence of disorder of the delocalized states is the presence at the initial time of normal (stable) modes only. In this case $U_n^{(0)}$ corresponds to the stable dynamics of the unperturbed problem and thus is bound in the index n: $U_n^{(0)} < \infty$ as $n \to \infty$. In its turn, the sufficient condition for the delocalized states is the *absence* of the (diffusion) U_n divergence: $U_n < \infty$ as $n \to \infty$. As soon as $U_n \to \infty$, as $n \to \infty$, this indicates the localized states.

It is easy to notice that the convergence or divergence of U_n is not dependent on the properties of the unperturbed solutions. The problem is reduced to a study of the asymptotic behaviour ($n \to \infty$) of the h_n coefficients in the linear transformation, eq.(33) [14]. This does not need calculation of the coefficients h_n but, by the means of analytical methods, analysis of the localization operator $H(z)$ as a function of the complex variable z. Therefore, the physical problem of the localized/delocalized states is reduced to the mathematical search for the poles of the function $H(z)$ of the complex variable [14, 15]. We do not go into details here; in particular, the diagrammic technique of the search for the poles was discussed in Appendix of Ref.[15].

In particular, it was shown [14, 15] that the localization operator $H(z)$ is a non-analytic function of the complex variable z. The unit circle $|z| = 1$ divides the complex plane into two analytic domains: the interior and exterior of the unit circle. The inverse Z-transform is quite generally defined via countour integrals in the complex plane

$$h_n = \frac{1}{2\pi i} \oint H(z) z^n \frac{dz}{z}. \tag{34}$$

This definition is only possible in an analytic domain and does not always represent a solution which can be physically interpreted [14, 15]. In this way, multiple solutions can result in the formal analysis of the problem. The first solution $H_+(z)$ describes the localized states. It is defined outside the unit circle and always exists. The second solution $H_-(z)$ describes delocalized states. It is defined inside the unit circle. The coexistence of the two solutions (if any) was physically interpreted [14, 15, 16] as the coexistence of two *phases* – an insulating and a metallic one.

Notice that the same result can be obtained using, instead of the total squared coordinate, eq.(16), the total squared momentum as a criterium of the diffusion dynamics

$$V_n = \int \frac{d^p \mathbf{k}}{(2\pi)^p} \langle |\psi_{n+1}(\mathbf{k}) - \psi_n(\mathbf{k})|^2 \rangle. \tag{35}$$

After simple transformations one gets

$$V(z) = H(z) V^{(0)}(z), \tag{36}$$

whose structure is similar to that of eq.(31), the definition of the localization operator $H(z)$ also retains, eq.(32), whereas $V^{(0)}(z)$ is the squared momentum of the unperturbed system.

The expression for the localization operator $H(z)$ has been derived by us earlier [14, 15]. However, the nontraditional *engineering language* was used (such as input/output signals, filter function, etc). As we demonstrated above, the derivation can be considerably simplified, since in the system of interacting modes the asymptotic behaviour of the total squared coordinate U_n serves as a natural indicator of the presence/absence of diffusion in the system's dynamics. Therefore, reformulation of the Schrödinger equation (quantum tight-binding model) in terms of the classical Hamiltonian map permits to retain the basic definitions of the alternative approach [14, 15, 16], but opens the additional possibility of a new interpretation of the results obtained earlier, which we discuss in the next Section.

III. THE FPU PROBLEM VS THE AL PROBLEM

A. Stability and thermalization

It is generally believed that an increase in space dimension greatly increases the system's stability with respect to disorder. Thus, there is without doubt the presence of a metal-insulator transition in the 3D case. It is believed that the effect of statistical fluctuations changes the regime at $D = 4$ [29, 30]; no phase transitions are expected for $D > 4$. The 2D system marks the *borderline* between high and low dimensions [31]. However, all these conclusions derive from the phenomenological scaling theory of localization [21]. The alternative point of view with different classification of high and low dimensions has been presented by us in Ref.[15]. In general, this confirms the system stability in higher dimensions.

An advantage of our interpretation of the AL in terms of classical dynamics of stochastically interacting oscillators is that it makes the statement on the relation between system stability and space dimension to be not so obvious. Indeed, for the energy range inside the old band $|E| \leq 2D$, where normal modes certainly exist, simultaneously the inverted modes with $|\mathcal{L}(\mathbf{k})| \geq 2$ are also always possible. Change of the space dimensions D affects the weights of these states, but their *complete* disappearance is impossible. That is, this problem can be resolved only by means of the exact analytical solution.

On the other hand, the *instability* mechanism for multi-dimensional systems ($D > 1$) in terms of oscillators is quite obvious. Even assuming that at the beginning only normal modes are excited, stochastic interaction inavoidably excites also neighboring, in particular, inverted modes. In other words, *thermalization* of all modes takes place. It is important to stress that *all* modes – normal and inverted ones – contribute to the localization operator $H(z)$, irrespective of which modes were excited in the beginning. The inverted mode dynamics in the classical phase space (p, q) corresponds to unbound trajectories which do not correspond to the delocalized states. However, an immediate conclusion suggests itself that all solutions of the dynamical problem – independent of the space dimension and disorder level – correspond only to the localized states. Such a paradox conclusion demonstrates clearly that the problem under consideration is counter-intuitive.

In our opinion, the *AL paradox* has much in common with the FPU problem [1, 3]. To show their close similarity, let us summarize here the main results.

Numerical simulations of a chain of harmonic oscillators coupled with a quadratic or cubic nonlinearity show that energy, initially placed in a low-frequency normal mode of the linear problem stay almost completely locked *within a few neighbor modes* (or *quasi-modes* [3]), instead of being distributed among *all modes of the system*. Recurrence of energy to the originally excited mode is also observed. The nonlinear effects are significant and cannot be neglected.

Two alternative explanations of the FPU paradox were suggested [3]): the integrability of nonlinear equations and dynamical (deterministic) chaos. The second approach points to the existence of a *stochasticity threshold* in the FPU problem. If the nonlinearity is below a stochasticity threshold, the dynamics of the system remains similar to the one of the unperturbed system for large time scales. For a strong nonlinearity the overlap of nonlinear resonances leads to a strong dynamical chaos, destroying the FPU effect. Namely in this case the intuitive thermalization occurs.

Therefore, in the standard FPU statement nonlinear effects play a *key role* being responsible for stochasticity: the motion of a nonlinear dynamical system even with few degrees of freedom can exhibit chaotic behavior. On the other hand, nonlinearity of the dynamics equations prevents their analytical analysis. A number of questions still remain open. In particular, the main results are obtained for systems with few degrees of freedom, the behavior of the system is not known in the thermodynamic limit, when the number of degrees of freedom goes to infinity.

In our interpretation of the Schrödinger equation in terms of the classical Hamiltonian map, stochasticity is introduced through on-site potentials, which are random variables. Therefore, there is no longer the need to solve nonlinear equations. For the Cauchy problem with fixed initial conditions, where the *causality principle* can be applied [14, 16], this problem can be solved *exactly analytically* (see Section II D), both for finite-size systems and its thermodynamic limit. Unlike the FPU problem with counter-intuitive solution, the classical interpretation of the AL problem is more complicated due to the unobvious dynamics of the inverted modes.

We will consider below the delocalized states in the quantum mechanical problem as statistically stable quasi-periodic motion, in terms of the classical Hamiltonian map, with excitations spreading only over a few neighbor modes (of the initially excited normal modes). Such a dynamics is bound. The localized states are interpreted respectively as diffusion

dynamics with statistically unbound trajectories. In the FPU problem this means thermalization with an excitation spreading over *all* modes.

B. Stochasticity threshold vs disorder threshold

As was noticed in Ref.[3], the existence of a *stochasticity threshold* in the FPU is the nonlinear effect. For a strong nonlinearity the overlap of nonlinear resonances leads to a dynamical chaos, destroying the FPU recurrence. As a result, fast convergence to thermal equilibrium arises. The problem of the nonlinearity prevents its detailed analytical study. The stochasticity threshold depends on the type of nonlinearity, space dimension; the thermodynamic limit is also unclear. Compared to this situation, the dynamical interpretation of the Schrödinger equation has obvious advantages permitting an exact analytical solution. It is expected that in the stochastic AL problem the relevant stochasticity threshold transforms into the *disorder threshold*.

When comparing the two problems, one has to keep in mind that the AL was formulated as a statistical problem with an ensemble of random potential realizations. Thus, it is convenient to reformulate the FPU as a statistical problem. Introducing the stochasticity parameter K (nonlinearity coefficient [26]), the type of dynamical trajectories is defined by the initial conditions. In other words, in the nonlinear dynamic problem the stochasticity parameter is not a unique factor determining the dynamics. For example, the behavior of the FPU system depends strongly on whether low- or high-frequency modes are initially excited [3]. The number of excited modes seems also to be important for the dynamics.

As is well known, in such problems the phase space is divided into regions with qualitatively different types of motion, and these regions are separated by barriers. If initial conditions were chosen in the region corresponding to a stable quasi-periodic motion, this dynamics corresponds to the recurrent behavior as in the FPU experiment and is classified as the dynamics below the stochasticity threshold. In another region an instability of motion exists for a wide range of the initial conditions (the dynamics above the stochasticity threshold). The value of the stochasticity parameter K determines the borders of these regions.

Let us now define some domain in phase space and an ensemble of the initial conditions therein. If for a given K a whole domain chosen falls into some region, all trajectories in

this ensemble reveal the same dynamics – stable quasi-periodic motion or dynamical chaos (single phase domain) – otherwise an ensemble reveals trajectories of different kinds (two-phase domain). In the latter case trivial *co-existence* of the two phases (or two *dynamics*, in a statistical sense) takes place. Change of the stochasticity parameter K in a given ensemble leads to the phase transitions. It is easy to show that in our statistical problem phase transitions from single-phase to hetero-phase (phase co-existence) dominate, and vice versa, since these transitions correspond to the boundary motion of the regions. Transitions from one single-phase system to another single-phase are also possible since variation in the K parameter in the phase space can induce spontaneous creation of new regions with a different dynamics.

The Schrödinger equation in terms of the classical Hamiltonian map does not depend so strongly on the initial conditions. In fact, these determine only the quantity defined by eq.(30), whereas existence of localized/delocalized states is defined entirely by the localization operator $H(z)$, eq.(32), which does not depend at all on the initial conditions [14, 15, 16]. The physical reason for this is obvious. The ensemble of different trajectories in the AL can be created already for fixed initial conditions by means of the ensemble of random potential realizations. For these realizations, even qualitatively different trajectories in the classical phase space occur. There is no reason to believe that the disorder parameter σ defines uniquely the trajectory types. It can be assumed that some random potentials (called *coherent realization*) correspond to the solutions $\psi_n(\mathbf{k})$ close to average values $\langle\psi_n(\mathbf{k})\rangle$ (the *delocalization* regime). For these realizations excitation of neighbor modes also occurs, however, at the next discrete-time steps n these modes return to an equilibrium position, $\psi_n(\mathbf{k}) = 0$ (the recurrent behavior). In other words, only their *virtual* dynamics around equilibrium with limited amplitude takes place. For other potential realizations (the *localization* regime) thermalization occurs and the recurrent behavior disappears. The main physical question – whether these two regimes have comparable statistical contributions – needs drawing of the phase diagram [14, 15, 16].

Since the detailed AL study in the thermodynamic limit for an arbitrary space dimension D has already been published by us [15], we restrict ourselves here to the interpretation of the result from the point of view of the disorder threshold. As was shown [15], for $D \geq D_0 = 4$ the spectrum of wave function fluctuations changes, as well as the convergence of the integral in eq.(32). The spatial dimension $D_0 = 4$ was also discussed in Ref.[29, 30], however, the

conclusion was drawn therein that this is an upper critical dimension for localization, so no phase transitions are expected for $D > 4$. In other words, no localized states can exist here. Since appearance of the localized states in the dynamical version of the Schrödinger equation (13) means *thermalization* (i.e. energy transfer from initially excited modes to all other modes), the analog of the above-mentioned result [30] in the FPU is a very strong statement on the existence of entirely recurrent states and no convergence to the thermal equilibrium in dynamical systems for $D > 4$. That is, the Gibbs statistics would not be applicable for high-dimensional systems. However, this statement is not based on an exact solutions and looks very suspicious to us. Thus, let us consider the alternative idea.

According to our Ref.[15], for $D \geq D_0 = 4$ the problem is fundamentally simplified: for all energies inside the old band $|E| \leq 2D$ (where only the delocalized states exist) there is a disorder threshold $\sigma_0(E)$. There is no thermalization for $\sigma < \sigma_0(E)$, but only delocalized states, characterized by the (formal) Lyapunov exponent $\gamma \equiv 0$. For $\sigma \geq \sigma_0(E)$ thermalization occurs, all states are exponentially localized with a certain $\gamma(\sigma, E)$. As noticed [14, 15, 16], the Lyapunov exponent γ can be treated in the AL problem as the *long-range order* parameter: the two different phases reveal different γ values, $\gamma \equiv 0$ (delocalized states) and $\gamma \neq 0$ (localized states, respectively). A sharp separation in the phase diagram of the localized and delocalized states recalls the second-order phase transition, where phases cannot coexist. However, the phase transition here is not of the second-order, since γ reveals step-like changes at the disorder threshold. As the space dimension D increases, the system stability increases with respect to disorder, but thermalization in principle *cannot* completely disappears.

For the case $2 \leq D \leq 3$ (low-dimensionial case [15]) the problem becomes more complicated; the *energy threshold* $E_0 = E_0(D)$ also arises. The delocalized states disappear even under infinitesimal disorder on the boundaries of the old band, $E_0 \leq |E| \leq 2D$. In other words, only thermalization is possible in this energy range. There is no analog of the FPU recurrence here. In the region $|E| \leq E_0$ the disorder threshold $\sigma_0(E)$ again appears; e.g. for $D = 2$ $E_0 = 2$ and $\sigma_0(E) = 2(1 - \sigma^2/E_0^2)^{1/4}$ [14]), but its sense changes. If disorder σ exceeds the threshold, only the localized states exist (full thermalization). As $\sigma < \sigma_0(E)$, the disorder parameter σ no longer separates uniquelly the localized and delocalized states, since *phase co-existence* takes place [14, 15, 16]. In other words, in the ensemble of different disorder potential realizations in this region *both* localized and delocalized solution can

arise with comparable probabilities. As a result of phase co-existence, phase transition in low-dimensional systems should be considered as a first-order transition. As was said above, this non-trivial result has a direct analogy in the statistical version of the FPU problem.

In the 1D case the analogy between the AL and FPU problems disappears; the Schrödinger equation corresponds here to a *single* oscillator only and thermalization has no longer a meaning. Notice, however, that historically the FPU problem arose during the numerical simulations of a one-dimensional chain of oscillators [1, 3]. The localization in 1D means diffusion excitation in one degree of freedom with specific disorder effects. This is not surprising: when presenting the Schrödinger equation in the form of eq.(13), one of the spatial coordinates in the D-dimensional system was interpreted as a discrete time variable, respectively, the Hamiltonian dynamics is treated for oscillator systems in a $p = D-1$ space dimension. That is, the AL problem in a space dimension D should be compared with the FPU with a lower space dimension, $p = D - 1$.

C. FPU recurrence vs delocalization

For the sake of illustration, we restrict ourself to the case of the band centre $E = 0$ for 2D system. For this particular case for the delocalized states ($H(z) = H_{-}(z)$) we calculated analytically [14] the inverse Z-transform, eq.(34), and found the coefficients h_n in eq.(33). Eq.(33) can be transformed, respectively:

$$U_n - U_n^{(0)} = 2\tan(\phi)\sum_{l=1}^{n-1} U_l^{(0)}\sin(2\phi(n-l)). \tag{37}$$

Eq.(37) is valid only for $\sigma \leq 2$, provided $2\sin(\phi) = \sigma$ [14].

It is easy to notice that the solution for a disordered system derives from that for the ordered system with the help of the sinusoidal modulation. Taking into account that the full squared coordinate $U_n^{(0)}$ is a sum of oscillating quantities (normal modes), solution for the perturbed problem U_n is a quasi-periodic motion. That is, one observes a direct analog of the recurrent behaviour in the FPU systems.

As was mentioned above, the 2D case for the AL corresponds to the 1D dynamics. On the other hand, the FPU paradox was established for the first time namely for the one-dimensional system [1, 2], and the result was considered as counter-intuitive. This is why our exact analytical study of the AL in the 2D case and the statement on the existence of the

delocalized states [14] proves once more a close similarity between the AL and FPU. Indeed, if the recurrent behavior is possible for the 1D FPU and this result is generally accepted as reliable, there are no strong grounds to reject our conclusion on the delocalized states in the 2D AL, since these states are analogous to the 1D quasi-periodic motion in FPU.

IV. CONCLUSION

The Anderson localization and Fermi-Pasta-Ulam problems are very complementary; each non-trivial and, as a rule, counter-intuitive result in one problem has its analog in another problem. In particular, a stable quasi-periodic motion (the recurrent behavior) in the FPU corresponds to the existence of the delocalized states in the AL problem. In contrast, the thermalization effect in FPU has an analog in the localized states in the AL. In general, we have shown here that a deep analogy between these two problems is possible, when we treat the quantum tight-binding model in terms of a classical Hamiltonian map.

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